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An X-ray study of DL-tyrosine hydrochloride

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Crystals of L-tyrosine hydrochloride have been studied for their structure by Srinivasan (1956, 1959). No work was reported on the crystal structure of the racimic form of tyrosine hydrochloride, $OHC_6H_4CH_2CH(NH_2)COOH.HCL$. Crystals of DL-tyrosine hydrochloride were grown from a saturated solution of DL-tyrosine in conc. hydrochloric acid after prolonged evaporation at about 50°C. As single crystals were not obtained, the Debye-Scherrer pattern of the micro-crystals have been studied and analysed.

The patterns were taken on an 11.48 cms diameter powder camera using CuK_α radiation, and the line positions were measured to an accuracy of 0.005 cm. The interplaner spacings obtained, were accurate up to 0.001Å near $2\theta = 62°$. Tests for higher crystal symmetries (Azàroff & Buerger 1958, Lipson 1949) of the observed data (table 1) showed that the crystal system was not either cubic, tetragonal, hexagonal or orthorhombic. Pairs of reflections were observed from the summations of Q $(10^4/d^2)$ values and the pattern has been indexed successfully for the monoclinic symmetry using formula :

$$Q_{hkl} = h^2Q_{100}+k^2Q_{010}+l^2Q_{001}+2hl(Q_{100}.Q_{001})^{\frac{1}{2}} \cos\beta^*.$$

Given indices 011 and 100 respectively to the first and fourth line, the second, third, fifth and sixth lines have been identified as 030, 002, 120 and 121 respectively where the constants $Q_{100} = 400$, $Q_{010} = 30.3$, $Q_{001} = 82$, $2(Q_{100}.Q_{001})^{\frac{1}{2}} \cos\beta^* = 40$ were obtained after refinement from higher orders of reflections.

Cell dimensions calculated from above constants, are $a = 5.03 \pm 0.003$, $b = 18.17 \pm 0.012$, $c = 11.11 \pm 0.007$Å, $\beta = 96°20'$. The unit cell is found reduced by Buerger's (1957) test. Density of these crystals, as determined with a small sp. gravity bottle is 1.40(5)$g.\ cm^{-3}$, and assuming $Z = 4$, the calculated density is 1.42 $g.cm^{-3}$. All possible indices within a discrepancy of $Q_{obs} \sim Q_{cal} = 8$, were calculated for each line and the conditions limiting possible reflections are :

hkl, no condition
*h*0*l*, $l = 2n$
0*k*0, no condition.

The probable space group is therefore P 2/c.

Table 1.

Intensity	d.Å	$10^4/d^2$(Obs)	$10^4/d^2$(Calc)	hkl
vs	9.509	111	112	011
w	6.067	272	273	030
w	5.539	326	328	002
vs	4.997	400	400	100
m	4.385	520	521	120
vs	3.943	643	643	121
			648	102
m	3.739	715	715	131
s	3.414	858	859	023
vs	3.357	887	885	140
m	3.095	1044	1048	113
vw	2.912	1179	1173	061
s	2.730	1342	1342	014
vs	2.595	1485	1485	070
vw	2.539	1551	1552	104
s	2.501	1599	1600	200
vw	2.414	1716	1721	220
m	2.341	1825	1825	134
			1829	063
vw	2.292	1904	1899	162
			1902	114
w	2.227	2016	2016	153
			2021	081
w	2.106	2255	2247	241
			2253	242
w	2.014	2465	2461	181
			2464	
w	1.958	2608	2608	213
vw	1.888	2805	2797	074
			2808	055
vw	1.850	2922	2923	135
w	1.786	3135	3135	145
			3141	065
vw	1.755	3247	3247	271
			3251	084
vw	1.695	3481	3482	193
vw	1.659	3633	3630	310
vw	1.589	3961	3961	332
vw	1.534	4250	4251	333
vw	1.506	4409	4404	0, 11, 3
			4411	137
vw	1.461	4685	4683	166
			4684	1, 11, 3
			4691	360; 0, 12, 2

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